

# Joint International Symposium

“Activation of Small Molecules - Gas Phase Clusters, Molecular Catalysts, Enzymes and Solid Materials”

February 20 – 23, 2011

Bildungszentrum Erkner, Seestraße 39, 15537 Erkner



## Highlights

- Unifying concepts of homogeneous, heterogeneous and enzymatic catalysis
- Experimental and computational studies on model catalysis, gas phase clusters and thin films in UHV
- Biomimetic and bio-inspired models for enzymes
- Materials design and synthesis for catalysis
- Detailed studies on complex reactions as oxidative dehydrogenation and oxidative coupling

## Discussion of results

- 12 years SFB 546 "Structure, Dynamics and Reactivity of Transition Metal Oxides"
- 3 years UniCat, mainly Research Areas A and C

## Program

- **Invited talks**  
E. Altmann (Yale), W. Goodman (Texas), H. Häkkinen (Finland), U. Heiz (TU M), D. Kolb (Ulm), T. Marks (Evanston, USA), H. Metiu (Santa Barbara), F. Neese (Bonn), D. Nocera (MIT), P. Stair (Evanston, USA), K. Wieghardt (Mülheim)
- **Overview lectures**  
J. Sauer (SFB 546) and M. Driess (UniCat)
- **Lectures**  
12 members of the SFB 546/UniCat
- **Poster sessions**

## Organiser

SFB 546  
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in cooperation with

UniCat  
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[www.chemie.hu-berlin.de/sfb546/Symposium2011/Symposium2011.html](http://www.chemie.hu-berlin.de/sfb546/Symposium2011/Symposium2011.html)

# **Joint International Symposium**

Collaborative Research Center 546  
Cluster of Excellence UniCat

## **Activation of Small Molecules**

**Gas Phase Clusters, Molecular Catalysts,  
Enzymes and Solid Materials**

**Erkner, February 20-23, 2011**

# List of Posters

No.	Authors	Poster Title
1	Gause, Hagemann, Küttner, Wöste, Werncke, Ohde, Limberg	Charge Reversal Experiments on oxovanadium(V) thiobisphenolates with 10 fs VIS-NIR Broadband Pulses & Building a systematic library for identification of Hydrocarbon Photoproducts
2	Burow, Wende, Claes, Jiang, Wlodarczyk, Sierka, Meijer, Lievens, Sauer, Asmis	Structures of cerium oxide cluster cations $Ce_mO_n^+$ in the gas phase from theory and experiment
3	Jiang, Wende, Claes, Bhattacharyya, Sierka, Meijer, Lievens, Sauer, Asmis	Electron distribution in partially reduced mixed metal oxide systems: Infrared spectroscopy of $Ce_mVnO_o^+$ gas phase clusters
4	Liu, Mohamed, Sauer	Selective oxidation of propene by vanadium oxide sites supported on silica
5	Uhlrich, Löffler, Yu, Yang, Shaikhutdinov, Freund	Reactivity of silica-supported vanadia/ceria model catalysts in methanol oxidation
6	Wolfram, Hamilton, Tzolova-Müller, Kröhnert, Trunschke, Schlögl	Synthesis of vanadium and titanium oxides on SBA-15 as catalysts for the oxidative de-hydrogenation of propane
7	Ovsitser, Beck, Schomäcker, Kondratenko	Improving of olefin selectivity in dehydrogenation of $C_3$ - $C_4$ alkanes over highly dispersed $VO_x$ species
8	Ohde, Limberg	From surface-inspired oxovanadium silsesquioxane models to active oxidation catalysts
9	Werncke, Limberg	Oxovanadium(V) Thiobisphenolates as Model Compounds for Supported $V_2O_5$ Employed in the Oxidative Dehydrogenation of Alkanes
10	Beck, Hamilton, Wohlgemuth, Trunschke, Schlögl, Schomäcker	The partial ethanol oxidation as model reaction for supported vanadia catalysts
11	Carrero, Wolfram, Trunschke, Schlögl, Schomäcker	Kinetics of Oxidative Dehydrogenation of Propane over $VO_x/TiO_y/SBA-15$ catalysts. "Looking for the ideal V/Ti ratio"
12	Harth, Möllmann, Berthold, Carrero, Schubert	Oxygen defect formation in $VO_x$ -catalysts – a support effect
13	Karslioglu, Kühlenbeck, Freund	Preparation of mixed molybdenum/titanium oxide layers
14	Primorac, Naschitzki, Kühlenbeck, Freund	Preparation of mixed vanadium/titanium oxide layers
15	Hucho, Wirsig	Strain fields and catalysis
16	Popa, Paier, Ganduglia-Pirovano, Sauer	The effect of the supporting oxide on the activity of vanadia/ceria catalysts
17	Gruber, Hermann	Selective Catalytic Reduction of NO with $NH_3$ at $V_2O_5(010)$ and Silica supported
18	Guo, Hermann, Hävecker, Gregoriades, Sauer, Trunschke, Schlögl	Analysis of Silica-Supported Molybdena by X-ray Absorption Spectroscopy: combined theoretical DFT cluster studies and NEXAFS measurements

No.	Authors	Poster Title
19	Unterberger, Kreiemeyer, Duncan, Bradley, Lerotholi, Window, Woodruff	Quantitative structural studies of titanium and vanadium oxide surfaces
20	Seifert, Schüller, Busch, Meyer, Winter	Structure of oxygen and ultrathin oxide films deposited on metal surfaces
21	Sicolo, Mohamed, Sauer, Gonchar, Risse, Freund	Differences in the Reactivity of Point Defects on MgO Surfaces: Interaction of CO with F-centers
22	Heitz, Aksu, Drieß	Quality MgO-based Catalysts Design by Single Source Precursor Approach
23	Kwapien, Sierka, Döbler, Sauer, Haertelt, Fielicke, Meijer	Vibrational spectroscopy of MgO clusters
24	Haertelt, Fielicke, Meijer, Kwapien, Sierka, Döbler, Sauer	Complexes of cationic MgO clusters
25	Greco, Bruschi, Bertini, Fantucci, Ryde, De Gioia	Cyanide ligands in [FeFe]-hydrogenases active site: dissecting their role in biological H <sub>2</sub> evolution
26	Mavlyankariev, Geske, Korup, Goldsmith, Schomäcker, Schlögl, Horn	Investigation of gas phase methane oxidative coupling by spatial profile measurements and microkinetic modeling
27	Beret, van Wijk, Ghiringhelli, Scheffler	Towards catalysis by free gold clusters in CO and O <sub>2</sub> atmosphere: an <i>ab initio</i> study
28	Fischer, Aksu, Driess, Thomas, Guiet, Perez, Lehmann, Frasca, Wollenberger	Mesoporous Transparent Conductive Bio-interfaces
29	Rábay, Teltewskoi, Jungton, Braun	C-H and N-H Activation Reactions at Ir and Rh: From Model Reactions to Catalysis
30	Butschke, Schwarz	Thermal C-H Bond Activation with Cationic [M(X)(bipy)] <sup>+</sup> – A Mechanistic Study
31	Kretschmer, Schlangen, Schwarz	Gas-Phase Monomethylation of Ammonia by "Bare" Zn(CH <sub>3</sub> ) <sup>+</sup> : An Unusual S <sub>N</sub> 2 Reaction with Atomic Zinc as a Leaving Group
32	Duric, Albrecht, Wiebalck, Tzschucke	Towards Artificial Photosystems: Ligandsynthesis and Model Systems
33	Enthaler, Fischer, Krackl, Epping, Weidner	Iron-catalyst supported on polyformamidines for C-C bond formations
34	Nowag, Keilitz, Thomas, Schomäcker, Haag	Dendritic Core-Multishell Architectures for the Stabilisation of Metal-Nanoparticle and their Application in Catalysis
35	Yao, Company, Herwig, Limberg, Driess	Reactivity of an Isolable Ni-Superoxo Complex: Dioxygenase-like Activity towards Selected Substrates and Monooxygenase-Like Activity in a Ni-O <sub>2</sub> -Fe system
36	Pffirmann, Limberg, Herwig, Stößer, Knispel, Braun, Metzinger	Exploring the Hydride Chemistry of $\beta$ -Diketiminato Nickel Complexes
37	Risch, Klingan, Lange, Ringleb, Kohlhoff, Fischer, Heidkamp, Chernev, Zaharieva, Aziz, Dau	X-ray absorption spectroscopy with soft and hard X-rays: Multi-edge analysis of a water-oxidizing cobalt film provides an exceptionally comprehensive picture
38	Schraut, Arbuznikov, Kaupp	Density-Functional Calculations of the EPR Parameters of the Oxygen-Evolving Complex of Photosystem II

No.	Authors	Poster Title
39	Reschke, Havelius, Horn, Haumann, Leimkühler	Investigations on the binding and insertion of Moco to molybdoenzymes in <i>Escherichia coli</i>
40	Klaumünzer, Banerjee, Saalf-rank	Calculation of Vibrational and Optical Spectra of Flavins and Flavoproteins
41	Yarman, Peng, Wu, Fischer, Gajovic-Eichelmann, Wollenberger, Hofrichter, Ullrich, Scheibner, Scheller	Direct electron transfer and substrate conversion by microperoxidase and peroxygenase in a biomimetic architecture
42	Arndt, Simon, Heitz, Berthold, Beck, Görke, Epping, Otremba, Aksu, Irran, Laugel, Horn, Driess, Schubert, Schomäcker	Update on Li/MgO as Catalyst for the Oxidative Coupling of Methane
43	Wilckens, Rüttinger, Kuse, Czekelius, Butschke, Schwarz	Gold-Catalyzed Heterofunctionalization of 1,4-Diynes
44	Schwarze, Keilitz, Dimroth, Nowag, Haag, Schomäcker	Recyclable Metal Catalysts for Hydrogenation Reactions
45	Dey, Mummy, Steinhilber, v. Klitzing, Lensen, Haag	Novel polymeric supports from the immobilization and stabilization of chemo- and biocatalysts as well as cells for catalytic reactions
46	Simon, Arndt, Jaso, Godini, Heldt, Wozny, Schomäcker, Schubert	Investigations of Phase Formation and Catalytic Activity of Na-W-Mn/SiO <sub>2</sub> Catalysts
47	Vuyyuru, Strasser	Heterogeneous & electro-catalytic conversion of biomass derived 5-hydroxymethylfurfural (HMF) into its oxidative products
48	Simon, Arndt, Schomäcker, Schubert, Dinse	Li-transition metal codoping of MgO - Defect chemistry, EPR spectroscopy and catalytic stability
49	Eppinger, Holst, Gordini, Jaso, Kraume, Steinbach, Arellano Garcia, Wozny	Different Aspects in Modeling and Design of Reactor Concepts for the Oxidative Coupling of Methane
50	Ranjbar Sahraie, Strasser, Lenz, Zebger, Fischer, Millo	Novel immobilization of O <sub>2</sub> -tolerant membrane bound hydrogenase, <i>Ralstonia eutropha</i> on self-assembled monolayer (SAM) modified gold electrode and high surface area materials for hydrogen production
51	Schwalbe	Extensive Mössbauer Studies on Iron Corrole-Complexes Attached to a Xanthene Scaffold and their Application in O-O Bond Activation
52	Feng, Ganduglia-Pirovano, Huo, Jiao, Sauer	Copper and gold clusters adsorption on $\gamma$ -alumina surfaces
53	Lublow, Zehl, Scorupska, Lewerenz, Fiechter	Self-Organized Nano-Architectures of Plasmonic Au-Particles for Photoelectrocatalysis
54	Fiechter, Bogdanoff, Ellmer, Kunst, Lewerenz, Ramirez, Kramm	Nanostructured Materials for Light-induced Water Splitting and Fuel Cells

# List of Speakers

Speakers	Title
<b>Eric Altman</b> (Yale School of Engineering & Applied Science, USA)	Applying Surface Science to Complex Transition Metal Oxide Catalysts
<b>Knut Asmis</b> (FHI Berlin, Germany)	Gas Phase Vibrational Spectroscopy of Transition Metal Oxide Clusters
<b>Siegfried Blechert</b> (TU Berlin, Germany)	Consecutive Catalysis
<b>Holger Dau</b> (FU Berlin, Germany)	Water oxidation - from photosynthesis to amorphous metal oxides
<b>Holger Dobbek</b> (HU Berlin, Germany)	Metalloenzymes in the bacterial life on carbon monoxide
<b>Matthias Driess</b> (TU Berlin, Germany)	Chemical & Biological Catalysis Unified: Aims, Unique Features and Selected Achievements of UniCat
<b>André Fielicke</b> (FHI Berlin, Germany)	Shedding IR light on gas phase clusters: structures and reactions
<b>Hans-Joachim Freund</b> (FHI Berlin, Germany)	Atom-scale description and control of complex surface structures
<b>Hannu Häkkinen</b> (University of Jyväskylä, Finland)	Survival stories of catalytic nanoscale gold: Clusters in gas phase, protected by ligands and supported by oxides
<b>Ulrich Heiz</b> (TU München, Germany)	Oxidation of CO on magnesia supported, partially oxidized Pd nano-clusters
<b>Raimund Horn</b> (FHI Berlin, Germany)	Model studies on Catalytic and Gas Phase Methane Oxidative Coupling
<b>Dieter Kolb</b> (Universität Ulm, Germany)	Tuning the catalytic properties of electrodes by surface strain
<b>Sergey Levchenko</b> (FHI Berlin, Germany)	Charged defects on oxide surfaces: formation energies and thermodynamics

<b>Speakers</b>	<b>Title</b>
<b>Christian Limberg</b> (HU Berlin, Germany)	From surface-inspired oxovanadium models to active catalysts for the oxidation of alcohols with O <sub>2</sub> and bio-mimetic sulfoxidations
<b>Tobin Marks</b> (Northwestern University, USA)	Oxides as Activators and Ligands for Organometallic Molecule-Derived Small-Molecule Catalysis
<b>Horia Metiu</b> (University of California, USA)	Doped oxides as catalysts for methane activation
<b>Frank Neese</b> (Universität Bonn, Germany)	Insight into C-H bond activation by nonheme iron centers from a combination of spectroscopy and quantum chemistry
<b>Niklas Nilius</b> (FHI Berlin, Germany)	Defects in transition and rare-earth metal oxides investigated with STM and DFT
<b>Daniel G. Nocera</b> (MIT, USA)	Solar Energy Conversion Catalysis: An Artificial Oxygen Evolving Complex Enables the Construction of an Artificial Leaf
<b>Joachim Sauer</b> (HU Berlin, Germany)	Structure and reactivity of transition metal oxides: gas phase, clusters, thin films, single crystals and supported catalysts
<b>Robert Schlögl</b> (FHI Berlin, Germany)	Oxidative dehydrogenation of propane: from model systems to high performance catalysts
<b>Reinhard Schomäcker</b> (TU Berlin, Germany)	The impact of support materials on the activity of vanadium oxide catalysts in oxidative dehydrogenation reactions
<b>Helmut Schwarz</b> (TU Berlin, Germany)	Homolytic C-H Bond Activation: The Role of Oxygen-Centered Radicals and Mechanistic Aspects
<b>Peter C. Stair</b> (Northwestern University, USA)	The Structure and Reactivity of Supported Vanadium Oxide
<b>Arne Thomas</b> (TU Berlin, Germany)	Catalysis with Porous Functional Materials
<b>Karl Wieghardt</b> (MPI Mülheim, Germany)	Coordination Chemistry with Radical Ligands: Where are the Valence Electrons?

Wednesday, February 23, 2011

	<b>Chairperson: M. Veronica Ganduglia-Pirovano</b>
08:45 – 09:30	<b>Hanu Häkkinen</b> Survival stories of catalytic nanoscale gold: Clusters in gas phase, protected by ligands and supported by oxides
09:30 – 10:00	<b>Niklas Nilius</b> Defects in transition and rare-earth metal oxides investigated with STM and DFT
10:00 – 10:30	<b>Coffee break</b>
	<b>Chairperson: Silke Leimkühler</b>
10:30 – 11:00	<b>Holger Dobbek</b> Metalloenzymes in the bacterial life on carbon monoxide
11:00 – 11:30	<b>André Fielicke</b> Shedding IR light on gas phase clusters: structures and reactions
11:30 – 12:00	<b>Christian Limberg</b> From surface-inspired oxovanadium models to active catalysts for the oxidation of alcohols with O <sub>2</sub> and biomimetic sulfoxidations
12:00	<b>Lunch, Departure</b>

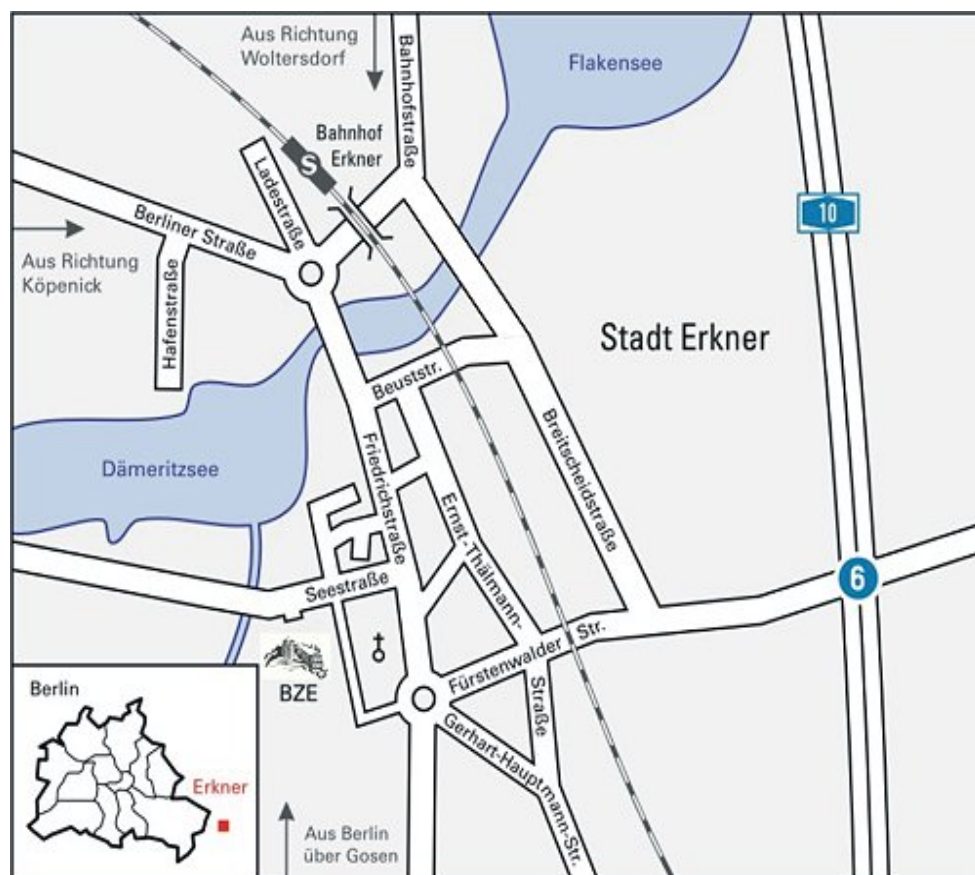
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**How to reach the BZE by Train:**

The RE1 to Erkner departs from all five large Berliner train stations Zoologischer Garten, Hauptbahnhof, Friedrichstraße, Alexanderplatz or Ostbahnhof (or the S-Bahn S3).



## Joint International Symposium

CRC 546  
 CoE UniCat

### Activation of Small Molecules Gas Phase Clusters, Molecular Catalysts, Enzymes and Solid Materials



**Erkner, February 20-23, 2011**

Sunday, February 20, 2011

16:30 – 17:00	<b>Coffee</b>
17:00 – 17:15	<b>Welcome: Hans-Joachim Freund</b>
	<b>Chairperson: Albrecht Goldmann</b>
17:15 – 18:00	<b>Matthias Driess</b> Chemical & Biological Catalysis Unified: Aims, Unique Features and Selected Achievements of UniCat
18:00 – 18:45	<b>Joachim Sauer</b> Structure and reactivity of transition metal oxides: gas phase, clusters, thin films, single crystals and supported catalysts
19:00 – 20:30	<b>Dinner</b>
20:30 – 22:00	<b>Poster arrangement, welcome drink</b>



Monday, February 21, 2011	
	<b>Chairperson: Thomas Braun</b>
08:45 – 09:30	<b>Daniel G. Nocera</b> Solar Energy Conversion Catalysis: An Artificial Oxygen Evolving Complex Enables the Construction of an Artificial Leaf
09:30 – 10:15	<b>Peter C. Stair</b> The Structure and Reactivity of Supported Vanadium Oxide
10:15 – 10:45	<b>Coffee break</b>
	<b>Chairperson: Martin Kaupp</b>
10:45 – 11:30	<b>Karl Wieghardt</b> Coordination Chemistry with Radical Ligands: Where are the Valence Electrons?
11:30 – 12:00	<b>Helmut Schwarz</b> Homolytic C–H Bond Activation: The Role of Oxygen-Centered Radicals and Mechanistic Aspects
12:00 – 12:30	<b>Arne Thomas</b> Catalysis with Porous Functional Materials
12:30 – 14:00	<b>Lunch</b>
	<b>Chairperson: Gerard Meijer</b>
14:00 – 14:45	<b>Ulrich Heiz</b> Oxidation of CO on magnesia supported, partially oxidized Pd nano-clusters
14:45 – 15:15	<b>Robert Schlögl</b> Oxidative dehydrogenation of propane: from model systems to high performance catalysts
15:15 – 15:45	<b>Reinhard Schomäcker</b> The impact of support materials on the activity of vanadium oxide catalysts in oxidative dehydrogenation reactions
15:45– 16:15	<b>Coffee break</b>
	<b>Chairperson: Karlheinz Schwarz</b>
16:15– 17:00	<b>Frank Neese</b> Insight into C-H bond activation by nonheme iron centers from a combination of spectroscopy and quantum chemistry
17:00– 17:30	<b>Sergey Levchenko</b> Charged defects on oxide surfaces: formation energies and thermodynamics
17:30– 18:00	<b>Raimund Horn</b> Model studies on Catalytic and Gas Phase Methane Oxidative Coupling
18:30– 20:00	<b>Dinner</b>
20:00 – 22:00	<b>Poster Session I (even No.)</b>

Tuesday, February 22, 2011	
	<b>Chairperson: Phil Woodruff</b>
08:45 – 09:30	<b>Eric Altman</b> Applying Surface Science to Complex Transition Metal Oxide Catalysts
09:30 – 10:15	<b>Dieter Kolb</b> Tuning the catalytic properties of electrodes by surface strain
10:15 – 10:45	<b>Coffee break</b>
	<b>Chairperson: Helmut Winter</b>
10:45 – 11:30	<b>Tobin Marks</b> Oxides as Activators and Ligands for Organometallic Molecule-Derived Small-Molecule Catalysis
11:30 – 12:00	<b>Holger Dau</b> Water oxidation – from photosynthesis to amorphous metal oxides
12:00 – 12:30	<b>Siegfried Blechert</b> Consecutive catalysis
12:30 – 14:00	<b>Lunch</b>
14:00 – 15:45	<b>Poster Session II (odd No.)</b>
15:45– 16:15	<b>Coffee break</b>
	<b>Chairperson: Uwe Kreibitz</b>
16:15– 17:00	<b>Horia Metiu</b> Doped oxides as catalysts for methane activation
17:00– 17:30	<b>Hans-Joachim Freund</b> Atom-scale description and control of complex surface structures
17:30– 18:00	<b>Knut Asmis</b> Gas Phase Vibrational Spectroscopy of Transition Metal Oxide Clusters
18:30– 20:00	<b>Dinner</b>

